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N-dimensional harmonic oscillator yields monotonic series for the mathematical constant π

R. LYNCH and H.A. MAVROMATIS
Physics Department, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia

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Abstract: Recently, Mavromatis (1990) has shown that the usual quantum mechanical ideas of matrix elements, expansion in complete sets, and the like, coupled to the three-dimensional harmonic oscillator problem, lead to an infinite set of series expansions for the mathematical constant π. In this paper his results are extended by considering a harmonic oscillator in a general space of N dimensions. It is found that in each *odd* dimension one obtains series for π, while in each *even* dimension, series for $1/\pi$.

Keywords: Series for π, N-dimensional harmonic oscillator.

1. Introduction

This paper describes an extension of earlier work [7] in which the usual quantum mechanical ideas of matrix elements, expansion in complete sets, and the like, coupled to the harmonic oscillator problem, lead to an infinite set of series expansions for the mathematical constant π. The results of the original investigation were obtained via three-dimensional harmonic oscillator wavefunctions; in this paper the scope of the technique is enlarged by considering a harmonic oscillator in a general space of N dimensions.

The impetus for undertaking the work to be described arose from a desire to more fully understand whether the connection between π and quantum mechanics expresses something deep and fundamental, or arises only from incidental considerations, such as symmetry. It was hoped, furthermore, that the almost embarrassing riches of series found in the original work might also prove to be somehow connected.

Neither of these aims have been fulfilled, but, nevertheless, some interesting results have been obtained. These encompass series for $1/\pi$, more diverse series for π, and, incidentally, expressions for the N-dimensional harmonic oscillator wavefunctions, which to the authors' knowledge have not appeared elsewhere.

2. Motivation

Consider the following definite integrals [6]:

$$\int_0^\infty x^{2n+1} \exp(-x^2)\, \mathrm{d}x = \tfrac{1}{2} n! = \tfrac{1}{2}\Gamma(n+1), \quad n = 0, 1, 2, \ldots, \tag{1}$$

and

$$\int_0^\infty x^{2n} \exp(-x^2)\, \mathrm{d}x = \frac{(2n-1)!!\pi^{1/2}}{2^{n+1}} = \tfrac{1}{2}\Gamma(n+\tfrac{1}{2}), \quad n = 0, 1, 2, \ldots, \tag{2}$$

where $(2n-1)!! \equiv 1 \cdot 3 \cdot \ldots \cdot (2n-1)$, $(-1)!! \equiv 1$, and $\Gamma(x)$ is the usual gamma function [6, p.933]. Looking at these two integrals, one of us (Mavromatis) noted that:

(i) the integrals in which x occurs as an odd power, i.e., equation (1), yield rational numbers as a result, while when x occurs as an even power, as in equation (2), the result involves the transcendental number π;

(ii) the integrals are of the sort encountered when working with the one-dimensional harmonic oscillator wavefunctions, for example, in obtaining the normalization of these.

Is there some way to combine these facts to obtain (a number of) series expansions for π?

3. Brief history of the computation of π

The answer to the question is, of course, an emphatic yes, and the point of this paper is to explore the general technique for finding these expansions. Before doing this, however, it is useful to set the problem in its historical perspective by briefly reviewing a variety of results obtained in the past, in the search for useful computational schemes for π. For a more detailed chronology, see [4]; for a recent note on the problem, see [8]. (Readers interested in algorithms which give very fast convergence, such as the AGM iteration (Arithmetic-Geometric Mean), see [1].)

In the ancient world π was often simply taken to be 3. Archimedes (ca. 240 B.C.) was the first to make a scientific attempt at evaluating π, by the so-called *classical method*. (See Fig. 1.) By 1630 A.D. improvements and extensions of the classical method led to a value of π accurate to 39 decimal places.

In 1650 A.D. the English mathematician John Wallis, by considering the integral $\int_0^1 (1-x^2)^{1/2}\, \mathrm{d}x$, found the infinite product representation

$$\pi = \frac{2(2 \cdot 2 \cdot 4 \cdot 4 \cdot 6 \cdot 6 \cdot 8 \cdot \ldots)}{1 \cdot 3 \cdot 3 \cdot 5 \cdot 5 \cdot 7 \cdot 7 \cdot \ldots}. \tag{3}$$

Although this result is not found to be useful in computing π, it will be seen to have interesting connections to the present work.

The modern approach of obtaining π by means of series expansions developed from the work of Newton, Leibnitz and the Scottish mathematician James Gregory, ca. 1670 A.D., resulting among others in the slowly convergent Gregory–Leibnitz series

$$\arctan 1 = \tfrac{1}{4}\pi = 1 - \tfrac{1}{3} + \tfrac{1}{5} - \tfrac{1}{7} + \cdots. \tag{4}$$

With the advent of computers and improved series expressions, computation of π to a million or

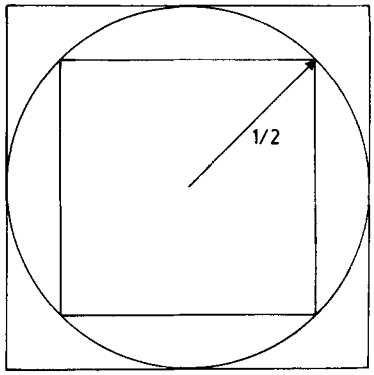

Fig. 1. Classical method for computing π. For a circle of unit diameter, the circumference lies between the perimeter of any inscribed regular polygon and any circumscribed regular polygon. In the figure the polygon is taken to be a square. The bounds are improved by taking the polygons to have more and more sides.

so places became feasible. Such computations, rather than being silly stunts, may serve a variety of purposes: to study the statistical properties of the digits of π, to provide speed or accuracy "benchmarks" for computers, and so on.

4. Two-dimensional harmonic oscillator

Before turning to the general N-dimensional treatment, for clarity of exposition we first give an example of the technique in a two-dimensional space. The illustration is chosen in two dimensions because the one-dimensional harmonic oscillator treatment turns out to be a special case of the technique, which will be taken up later in this paper; as noted above, the three-dimensional harmonic oscillator method has already been described in previous work [7].

The harmonic oscillator Hamiltonian is taken to be

$$H = \tfrac{1}{2}(\boldsymbol{p}\cdot\boldsymbol{p} + \boldsymbol{r}\cdot\boldsymbol{r}), \tag{5}$$

where $\boldsymbol{r} = (x_1, x_2)$ and $\boldsymbol{p} = (p_1, p_2)$. In the coordinate representation we make the operator replacements $x_1 \to x_1$, $x_2 \to x_2$, $p_1 \to -\mathrm{i}\partial/\partial x_1$, $p_2 \to -\mathrm{i}\partial/\partial x_2$. The Schrödinger equation for the wavefunction $\Psi(\boldsymbol{r})$ is

$$\nabla_2^2 \Psi(\boldsymbol{r}) + [2E - r^2]\Psi(\boldsymbol{r}) = 0, \tag{6}$$

where $\nabla_2^2 \equiv \partial^2/\partial x_1^2 + \partial^2/\partial x_2^2$, and $r \equiv (\boldsymbol{r}\cdot\boldsymbol{r})^{1/2}$.

As will be shown in Section 6 of this paper, imposing the usual conditions that $\Psi(\boldsymbol{r})$ be single-valued and finite everywhere, and normalized to unity—$\int \mathrm{d}^2\boldsymbol{r}\Psi^*(\boldsymbol{r})\Psi(\boldsymbol{r}) = 1$—it is found that (6) has solutions only for the *eigenvalues*

$$E_{nl} = 2n + l + 1, \tag{7}$$

where n and l may only assume nonnegative *integral* values, $n, l = 0, 1, 2, \ldots,$ The corresponding *eigenfunctions* are found to be (ϕ is the usual polar angle):

$$\Psi_{nl}(\boldsymbol{r}) = \left[\frac{(n+l)!}{\pi n!}\right]^{1/2}\left[\frac{r^l \exp(-\frac{1}{2}r^2)}{l!}\right] {}_1F_1(-n;\, l+1;\, r^2)\exp[\mathrm{i}l\phi]. \tag{8}$$

Here ${}_1F_1(a;\ c;\ z)$ is the *confluent hypergeometric function* [9]:

$$ {}_1F_1(a;\ c;\ z) = \sum_{p=0}^{\infty} \frac{\Gamma(a+p)\Gamma(z)z^p}{\Gamma(p)\Gamma(c+p)} = 1 + \frac{az}{c1!} + \frac{a(a+1)z^2}{c(c+1)2!} + \cdots. \tag{9} $$

The series for ${}_1F_1$ terminates, becoming a polynomial, for the condition mentioned above, i.e., n takes on only nonnegative integral values.

The reader may find (8) more familiar when written in terms of the *associated Laguerre polynomials* $L_n^a(x)$, where [9, p.208 f] $L_n^a(x) = (\Gamma(n+a+1)^2/[\Gamma(n+1)\Gamma(a+1)])\ {}_1F_1(-n;\ a+1;\ x)$:

$$ \Psi_{nl}(\boldsymbol{r}) = \left[\frac{n!}{\pi\,(n+l)!^3}\right]^{1/2} r^l \exp(-\tfrac{1}{2}r^2) L_n^l(r^2) \exp(\mathrm{i}l\phi). \tag{8$'$} $$

In Dirac notation the eigenvectors may be written as $|n,\ l\rangle$. Consider the matrix element $\langle n,\ l|r^2|n,\ l\rangle$. Inserting a complete set of states one may write

$$ \langle n,\ l|r^2|n,\ l\rangle = \sum_{n',l'} |\langle n,\ l|r|n',\ l'\rangle|^2. \tag{10} $$

Next use the quantum mechanical virial theorem [9, p.168] which in the present case says

$$ \langle n,\ l|\boldsymbol{r}\cdot\boldsymbol{r}|n,\ l\rangle = \langle n,\ l|\boldsymbol{p}\cdot\boldsymbol{p}|n,\ l\rangle = \langle n,\ l|H|n,\ l\rangle = E_{nl}. \tag{11} $$

Thus the left-hand side of equation (10) becomes $2n+l+1$.

By the orthogonality of the functions $\exp(\mathrm{i}l\phi)$ it is obvious that only terms for which $l'=l$ contribute to the right-hand side of equation (10); furthermore, under these conditions all the terms are real. Now defining

$$ A_{n'}^{(n,l)} \equiv \frac{\langle n,\ l|r|n',\ l\rangle}{\pi^{1/2}} \tag{12} $$

(the reason for the factor of $\pi^{1/2}$ will become clear shortly), we then may write

$$ \frac{1}{\pi} = \frac{1}{2n+l+1} \sum_{n'=0}^{\infty} \left(A_{n'}^{(n,l)}\right)^2. \tag{13} $$

Shifting back to the coordinate representation, and using the explicit wavefunctions in equation (8), one finds that

$$ A_{n'}^{(n,l)} = \frac{2}{l!^2}\left[\frac{(n+l)!(n'+l)!}{\pi\, n!\, n'!}\right]^{1/2} \times \int_0^{\infty} \mathrm{d}r\, r^{2l+2} \exp(-r^2)\, {}_1F_1(-n;\ l+1;\ r^2)\, {}_1F_1(-n';\ l+1;\ r^2). \tag{14} $$

In equation (14) each of the ${}_1F_1$ factors is a polynomial in r^2 (since as noted the series defining the confluent hypergeometric function (9) terminates when the first argument in the function is a negative integer). Thus the integral in equation (14) consists of a sum of terms of the form of equation (2), involving *even* powers of the variable of integration, for each of which a factor of $\pi^{1/2}$ is obtained, canceling the factor of $1/\pi^{1/2}$ in $A_{n'}^{(n,l)}$. Hence all the $(A_{n'}^{(n,l)})^2$ are rational numbers and equation (13) then gives a series expression for $1/\pi$, which is the desired result.

It is interesting to note that utilizing the technique with the two-dimensional harmonic oscillator yields a series expansion for $1/\pi$, while the original work [7] in a three-dimensional space gave a series for π. Later in this paper we will establish the general result that the method yields a series expansion for π in each *odd* dimension, and an expansion for $1/\pi$ in each *even* dimension.

In the Appendix of this paper we will also carry through the program mentioned above, and obtain a general expression for $A_{n'}^{(n,l)}$ in any dimension, which may be used to evaluate the rather forbidding-looking expression in equation (14). However, let us here consider the special case $n = l = 0$. For these values one finds

$$A_{n'}^{(0,0)} = \frac{2}{\pi^{1/2}} \int_0^\infty \mathrm{d}r\, r^2 \exp(-r^2)\, {}_1F_1(-n'; 1; r^2). \tag{15}$$

Working out the terms $n' = 0, 1, 2, \ldots$ using the definition of ${}_1F_1(a;\, c;\, z)$ and equation (2) one obtains

$$\begin{aligned} &A_0^{(0,0)} = \tfrac{1}{2}, \qquad A_1^{(0,0)} = -\tfrac{1}{4}, \qquad A_2^{(0,0)} = -\tfrac{1}{16}, \\ &A_3^{(0,0)} = -\tfrac{1}{32}, \qquad A_4^{(0,0)} = -\tfrac{5}{256}, \ldots, \end{aligned} \tag{16}$$

so that the series for $1/\pi$—equation (13)—becomes

$$\frac{1}{\pi} = \frac{1}{4} + \frac{1}{16} + \frac{1}{256} + \frac{1}{1024} + \frac{25}{65536} + \cdots, \qquad n,\ l = 0. \tag{17}$$

As is shown subsequently the general term in this particular series is $\Gamma(n' - \frac{1}{2})^2/4(n'!)^2\Gamma(-\frac{1}{2})^2$ and for large n' this goes as $(1/16\pi)n'^{-3}$.

Examining this series (or indeed from the form of (13)) it is apparent that the series is *monotonic*, i.e., all terms are positive. This means that such expansions will converge much more quickly than alternating series such as that of Gregory–Leibnitz (equation (4)). The rapid convergence is shown by comparing the value of the left-hand side of (14), $1/\pi = 0.31831\ldots$, to the sequence of partial sums of the right-hand side: 0.25, 0.3125, 0.31641..., 0.31738..., 0.31776.... The convergence properties of this type of series are considered in more detail in [7].

Another interesting feature of the general series expansions of this paper is found by considering the leading terms ($n' = 0$) of the expansions for $n = 0$ but arbitrary l. In this case the expression given in (14) is found quite easily, using (2), and the form of the leading term is

$$\frac{\left[A_0^{(0,l)}\right]^2}{l+1} = \frac{\left[(2l+1)!!\right]^2}{l!(l+1)!2^{2l+2}}. \tag{18}$$

Writing these out for $l = 0, 1, 2, \ldots$ one finds

$$\begin{aligned} l=0:&\quad \frac{1}{\pi} = \frac{1}{4} + \cdots = \frac{1}{2}\cdot\frac{1}{2} + \cdots, \\ l=1:&\quad \frac{1}{\pi} = \frac{9}{32} + \cdots = \frac{1}{2}\cdot\frac{1\cdot 3\cdot 3}{2\cdot 2\cdot 4} + \cdots, \\ l=2:&\quad \frac{1}{\pi} = \frac{75}{256} + \cdots = \frac{1}{2}\cdot\frac{1\cdot 3\cdot 3\cdot 5\cdot 5}{2\cdot 2\cdot 4\cdot 4\cdot 6} + \cdots, \\ &\quad \cdots \end{aligned} \tag{19}$$

We see that the leading terms are just successive approximations to the Wallis infinite product result—equation (3)—apparently a deep and somehow satisfying connection.

Finally, reconsidering (10) one might inquire whether new results might be obtained by exploring matrix elements involving higher powers of r. The method clearly could be used for higher *even* powers of r, say r^{2M}, by the identity $r^{2M} = r^M \cdot r^M$, but this has not been explored for $M > 1$, and perhaps will form the basis for a future investigation.

5. N-dimensional harmonic oscillator wavefunction

We now turn to the general case of N dimensions, first deriving an expression for the wavefunctions of the N-dimensional harmonic oscillator, which to the authors' knowledge is not given elsewhere.

The Hamiltonian is still given by equation (5) but now $\boldsymbol{r} = (x_1, x_2, \ldots, x_N)$ and $\boldsymbol{p} = (p_1, p_2, \ldots, p_N)$. Going to the coordinate representation yields the N-dimensional Schrödinger equation

$$\nabla_N^2 \Psi(\boldsymbol{r}) + [2E - r^2]\Psi(\boldsymbol{r}) = 0, \tag{20}$$

where $\nabla_N^2 = \partial^2/\partial x_1^2 + \partial^2/\partial x_2^2 + \cdots + \partial^2/\partial x_N^2$. In view of the symmetry of the problem we would like to write the wavefunction as the product of a radial part and an "angular" part. This may be accomplished by using the results given in a monograph [10]. Introduce a system of coordinates $\boldsymbol{\xi} = (\xi_1, \xi_2, \ldots, \xi_N)$ for points on the unit hypersphere ($\boldsymbol{\xi} \cdot \boldsymbol{\xi} = 1$). Then $\boldsymbol{r} = r\boldsymbol{\xi}$ and it is shown that one can write

$$\nabla_N^2 = \frac{\partial^2}{\partial r^2} + \frac{N-1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\nabla_N^{*2}, \tag{21}$$

where ∇_N^{*2} contains only "angular" derivatives. There exists a set of $\mathcal{N}(N, l)$ linearly independent "spherical harmonics" $S_{lm}(\boldsymbol{\xi})$, which are polynomials of degree l in $\boldsymbol{\xi}$. Here the index m runs over the set of values 0, 1, 2, ..., $\mathcal{N}(N, l)$, where

$$\mathcal{N}(N, l) = \begin{cases} \dfrac{(2l+N-2)(l+N-3)!}{l!(N-2)!}, & l \geqslant 1, \\ 1, & l = 0, \end{cases} \tag{22}$$

where $N \geqslant 2$. The $S_{lm}(\boldsymbol{\xi})$ satisfy

$$\nabla_N^{*2} S_{lm}(\boldsymbol{\xi}) + l(l+N-2)S_{lm}(\boldsymbol{\xi}) = 0. \tag{23}$$

Any function defined on the unit hypersphere may be expanded in terms of the $S_{lm}(\boldsymbol{\xi})$, just as with ordinary spherical harmonics. Thus writing $\Psi(\boldsymbol{r}) = R(r)S_{lm}(\boldsymbol{\xi})$, one finds upon separation of the Schrödinger equation that $R(r)$ satisfies

$$\left[\frac{d^2}{dr^2} + \frac{N-1}{r}\frac{d}{dr} - \frac{l(l+N-2)}{r^2} + (2E - r^2)\right]R(r) = 0. \tag{24}$$

The solution to this equation is readily found by setting $R(r) = \phi(r)/r^{(N-l)/2}$, after which one obtains the equation

$$\left[\frac{d^2}{dr^2} - \frac{(l + \frac{1}{2}N - \frac{3}{2})(l + \frac{1}{2}N - \frac{3}{2} + 1)}{r^2} + (2E - r^2)\right]\phi(r) = 0. \tag{25}$$

This equation is almost identical to one encountered in the solution of the three-dimensional harmonic oscillator problem [2], and it is thus found that the radial wavefunctions are given by

$$R_{nl}(r)=\left[\frac{2\Gamma(n+l+\frac{1}{2}N)}{n!}\right]^{1/2}\left[\frac{r^l\exp(-\frac{1}{2}r^2)}{\Gamma(l+\frac{1}{2}N)}\right]{}_1F_1(-n;\ l+\tfrac{1}{2}N;\ r^2), \tag{26}$$

which belong to the energy eigenvalue

$$E_{nl}=(2n+l+\tfrac{1}{2}N), \tag{27}$$

whose eigenfunction is $\Psi_{nlm}(\boldsymbol{r})=R_{nl}(r)S_{lm}(\boldsymbol{\xi})$. The $R_{nl}(r)$ are normalized according to

$$\int_0^\infty R_{nl}(r)R_{n'l}(r)r^{N-1}\,\mathrm{d}r=\delta_{nn'}. \tag{28}$$

In terms of the associated Laguerre functions, $R_{nl}(r)$ may be written as

$$R_{nl}(r)=\left[\frac{2n!}{\Gamma(n+l+\frac{1}{2}N)^3}\right]^{1/2}r^l\exp(-\tfrac{1}{2}r^2)L_n^{l+N/2-1}(r^2),\quad N>1. \tag{26'}$$

We note in passing that in all dimensions the harmonic oscillator eigenvalues may be labeled by just two quantum numbers n and l, which take on nonnegative integral values (n, $l=0, 1, 2, \ldots$). The eigenfunctions are labeled by an additional index m and each energy level corresponding to a given value of n, l is $\mathcal{N}(N, l)$-fold degenerate.

6. General result for N dimensions

With these wavefunctions in hand, the general result for N dimensions may now be pursued. Following the procedure of Section 4 one finds

$$\pi=\frac{1}{(2n+l+\frac{1}{2}N)}\sum_{n'=0}^{\infty}\left(A_{n'}^{(n,l)}\right)^2,\quad N\text{ odd},\ N\neq 1, \tag{29}$$

and

$$\frac{1}{\pi}=\frac{1}{(2n+l+\frac{1}{2}N)}\sum_{n'=0}^{\infty}\left(A_{n'}^{(n,l)}\right)^2,\quad N\text{ even}. \tag{30}$$

Here

$$A_{n'}^{(n,l)}\equiv\begin{cases}\pi^{1/2}\langle n,\ l,\ m\,|\,r\,|\,n',\ l,\ m\rangle, & N\text{ odd},\ N\neq 1,\\ \dfrac{\langle n,\ l,\ m\,|\,r\,|\,n',\ l,\ m\rangle}{\pi^{1/2}}, & N\text{ even}.\end{cases} \tag{31}$$

In equations (29) and (30) the general sum over the complete set $|n',\ l',\ m'\rangle$ has been reduced to a sum only over n', since r is a scalar operator which imposes the constraints $l=l'$, $m=m'$. Moreover for this operator the m-dependent functions S_{lm} may be integrated out so that the right-hand sides of equation (31) are independent of m, and this has been anticipated in writing $A_{n'}^{(n,l)}$ with no m-dependence. Finally, the special case $N=1$ will be treated separately in Section 7.

It is not terribly difficult to obtain a closed result for the matrix element $\langle n, l, m | r | n', l, m\rangle$, but as the derivation is somewhat complicated, it is relegated to the Appendix. The general result, valid in all dimensions except $N = 1$, is

$$\langle nlm | r | n'lm\rangle = (-1)^{n'}\left[\frac{\Gamma(n+l+\frac{1}{2}N)}{n!\,n'!\,\Gamma(n'+l+\frac{1}{2}N)}\right]^{1/2}\frac{\Gamma(l+\frac{1}{2}N+\frac{1}{2})}{\Gamma(l+\frac{1}{2}N)}\frac{\Gamma(\frac{3}{2})}{\Gamma(\frac{3}{2}-n')}$$
$$\times {}_3F_2(-n,\, l+\tfrac{1}{2}N+\tfrac{1}{2},\, \tfrac{3}{2};\, l+\tfrac{1}{2}N,\, \tfrac{3}{2}-n';\, 1), \quad N \neq 1. \tag{32}$$

Here the ${}_3F_2$ function is one of a class of functions known as *generalized hypergeometric series* [6, p.1045], defined by

$$\begin{aligned} &{}_pF_q(\alpha_1, \alpha_2, \ldots, \alpha_p;\, \beta_1, \beta_2, \ldots, \beta_q;\, z) \\ &= 1 + \frac{\alpha_1\alpha_2\cdots\alpha_p z}{\beta_1\beta_2\cdots\beta_q 1!} + \frac{\alpha_1(\alpha_1+1)\alpha_2(\alpha_2+1)\cdots\alpha_p(\alpha_p+1)z^2}{\beta_1(\beta_1+1)\beta_2(\beta_2+1)\cdots\beta_q(\beta_q+1)2!} + \cdots. \end{aligned} \tag{33}$$

Taking explicit wavefunctions, equation (32) can also be written as

$$\begin{aligned} &\int_0^\infty \exp(-x)x^{a+1/2}L_n^a(x)L_{n'}^a(x)\,\mathrm{d}x \\ &= \frac{\Gamma(a+n+1)^2\Gamma(a+n'+1)\Gamma(a+\frac{3}{2})\Gamma(n'-\frac{1}{2})}{n!\,n'!\,\Gamma(a+1)\Gamma(-\frac{1}{2})} \\ &\quad\times {}_3F_2(-n,\, a+\tfrac{3}{2},\, \tfrac{3}{2};\, a+1,\, \tfrac{3}{2}-n';\, 1), \end{aligned}$$

which to the authors' knowledge is a new result of some interest.

If one studies equation (32) somewhat it will be seen that if the factor $\Gamma(l+\frac{1}{2}N+\frac{1}{2})/\Gamma(l+\frac{1}{2}N)$ is separated off, all other factors (when squared) will combine to give a rational number. One can easily show that

$$\frac{\Gamma(l+\frac{1}{2}N+\frac{1}{2})}{\Gamma(l+\frac{1}{2}N)} = \begin{cases} \dfrac{(l+\frac{1}{2}N-\frac{1}{2})!\,2^{l+(N-1)/2}}{(2l+N-2)!!\,\pi^{1/2}}, & N \text{ odd}, \\[2ex] \dfrac{(2l+N-1)!!\,\pi^{1/2}}{2^{l+N/2}(l+\frac{1}{2}N-1)!}, & N \text{ even}, \end{cases} \tag{34}$$

so that a factor $\pi^{-1/2}$ or $\pi^{1/2}$ is produced depending on whether N is odd or even, respectively. These factors of $\pi^{1/2}$ cancel those introduced in the definition of the $A_{n'}^{(n,l)}$ in equations (29) and (30), and in all dimensions ($N > 1$) produce monotonic series for π or $1/\pi$, all of whose terms are rational numbers.

Equations (29)–(32) taken together are the central result of this paper; being quite general these equations are perhaps understandably somewhat complex. In the special case $n = 0$, however, the ${}_3F_2$ function becomes unity, and one finds after some work that if N is odd, $N \neq 1$,

$$\begin{aligned} \pi &= \frac{(l+\frac{1}{2}N-\frac{1}{2})!^2\,2^{2l+N}}{(2l+N)!!\,(2l+N-2)!!} \\ &\quad\times\left\{1 + \frac{1}{4(l+\frac{1}{2}N)} + \frac{1}{32(l+\frac{1}{2}N)(l+\frac{1}{2}N+1)}\right. \\ &\quad\left. + \frac{3}{128(l+\frac{1}{2}N)(l+\frac{1}{2}N+1)(l+\frac{1}{2}N+2)} + \cdots\right\}, \end{aligned} \tag{35}$$

while if N is even,

$$\frac{1}{\pi}=\frac{(2l+N-1)!!^2}{(l+\frac{1}{2}N)!\,(l+\frac{1}{2}N-1)!\,2^{2l+N}}$$
$$\times\left\{1+\frac{1}{4(l+\frac{1}{2}N)}+\frac{1}{32(l+\frac{1}{2}N)(l+\frac{1}{2}N+1)}\right.$$
$$\left.+\frac{3}{128(l+\frac{1}{2}N)(l+\frac{1}{2}N+1)(l+\frac{1}{2}N+2)}+\cdots\right\}. \tag{36}$$

The relations $\Gamma(n+1)=n\Gamma(n)$ and $\Gamma(z)/\Gamma(z-n)=(-1)^n\Gamma(-z+n+1)/\Gamma(-z+1)$ [3;6, p.937] may prove useful in obtaining these. One notes that the expression in equation (18) is just the leading term of the expansion (36) for the special case $N=2$.

It is also interesting to observe that in equations (35) and (36) increasing the dimension N by two units is equivalent to increasing l by one unit.

Finally, one can readily see that as $N\to\infty$, the expressions in braces in equations (35) and (36) go to unity. The leading terms are found to become Wallis's product ratio (or its inverse) (equation (3)). Thus Wallis' expression can be identified with the leading terms (or their inverses) in the expansions for π (or $1/\pi$) for $n=0$, in the limit as N goes to infinity.

In equations (35) and (36) the n'th terms ($n'=0, 1, 2, \ldots$) in the parentheses are given by $\Gamma(l+\frac{1}{2}N)\Gamma(n'-\frac{1}{2})^2/[n'!\,\Gamma(n'+l+\frac{1}{2}N)\Gamma(-\frac{1}{2})^2]$. For large n' one notes (using $\lim_{z\to\infty}\Gamma(z+a)/\Gamma(z+b)\to z^{a-b}$) that this term goes as $[\Gamma(l+\frac{1}{2}N)/\Gamma(-\frac{1}{2})^2]n'^{-2-l-N/2}$, showing that the rate of convergence improves as N, l increase.

7. One-dimensional harmonic oscillator result

Even though the case $N=1$ has been excluded in the derivation above, it is found that plugging in $N=1$, $l=0$ into equations (29), (31) and (32) results in the series

$$\pi=\frac{1}{4\Gamma(\frac{3}{2})}\sum_{n'=0}^{\infty}\left[\frac{\Gamma^2(n'-\frac{1}{2})}{\Gamma(n'+\frac{1}{2})n!}\right]^2=2+1+\frac{1}{12}+\frac{1}{40}+\frac{5}{448}+\cdots. \tag{37}$$

This is puzzling since if one goes through the steps of the technique as given above one does not obtain a series for π. (This will be left as an exercise for the reader.)

However, if one goes through the derivation with $|x|^2=|x|\cdot|x|$ instead, then one finds

$$\pi=\frac{1}{(n+\frac{1}{2})}\sum_{n'=0}^{\infty}(A_{n'}^{n})^2, \tag{38}$$

where

$$A_{n'}^{n}\equiv\pi^{1/2}\langle n|\,|x|\,|n'\rangle=\pi^{1/2}\int_{-\infty}^{\infty}|x|\phi_n(x)\phi_{n'}(x)\,\mathrm{d}x. \tag{39}$$

Here $\phi_n(x)$ are the usual one-dimensional harmonic oscillator wavefunctions [9, p.61]

$$\phi_n(x)=[2^n n!\,\pi^{1/2}]^{-1/2}\exp(-\tfrac{1}{2}x^2)H_n(x), \tag{40}$$

with the normalization $\int_{-\infty}^{\infty}\phi_n(x)\phi_{n'}(x)\,\mathrm{d}x=\delta_{nn'}$, where the $H_n(x)$ are Hermite polynomials of order n. For $n=0$ one recovers the series (37). Here again the leading term of the $n=0$ series, i.e., 2, is just the lowest order approximation to Wallis's product in (3).

8. Summary and conclusions

We have thus managed to develop a simple observation about the properties of some standard integrals (Section 2) into a doubly-infinite set (i.e., dependent on two parameters n, $l=0, 1, 2, \ldots$) of monotonic series for π or $1/\pi$ in every dimension N. Along the way we have had to obtain the general wavefunctions for the N-dimensional harmonic oscillator, an interesting problem in itself. The technique calls upon the quantum mechanical ideas of matrix elements, expansion in complete sets, and so on, to give a result in pure mathematics. The series expansions that are found are seen to be quickly convergent, a property due to their being monotonic, and perhaps also linked to the connection with the Wallis infinite product expansion of π.

In working with these series the authors have been struck by the incredible richness of the material studied, where a myriad of subtopics suggest themselves at each level of development. Perhaps the reader will also become interested, and explore some of these avenues of investigation.

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Appendix

Substituting the wavefunctions of (26) one finds for the basic matrix element:

$$\begin{aligned}&\langle nlm \,|\, r \,|\, n'lm\rangle\\ &= \frac{2}{\Gamma^2(l+\frac{1}{2}N)}\left[\frac{\Gamma(n+l+\frac{1}{2}N)\Gamma(n'+l+\frac{1}{2}N)}{n!n'}\right]^{1/2}\\ &\quad\times\int_0^\infty \mathrm{d}r\,r^{2l+N}\exp(-r^2)\,{}_1F_1(-n;\, l+\tfrac{1}{2}N;\, r^2)\,{}_1F_1(-n';\, l+\tfrac{1}{2}N;\, r^2).\end{aligned} \tag{41}$$

The integral does not appear to be one listed in the usual tabulations.

We proceed by plugging in the definition of the ${}_1F_1$ functions in (9) to obtain

$$\begin{aligned}&\langle nlm \,|\, r \,|\, n'lm\rangle\\ &= \frac{2}{\Gamma^2(l+\frac{1}{2}N)}\left[\frac{\Gamma(n+l+\frac{1}{2}N)\Gamma(n'+l+\frac{1}{2}N)}{n!n'!}\right]^{1/2}\\ &\quad\times\sum_{p=0}^{n}\sum_{p'=0}^{n'}\frac{\Gamma(-n+p)\Gamma(l+\frac{1}{2}N)\Gamma(-n'+p')\Gamma(l+\frac{1}{2}N)}{\Gamma(-n)\Gamma(l+\frac{1}{2}N+p)p!\,\Gamma(-n')\Gamma(l+\frac{1}{2}N+p')p'!}\\ &\quad\times\int_0^\infty \mathrm{d}r\,r^{2l+N+2p+2p'}\exp(-r^2).\end{aligned} \tag{42}$$

The integral in this equation is just that of equations (1) and (2), and one finds easily

$$\int_0^\infty \mathrm{d}r\, r^{2(l+N/2+p+p')} \exp(-r^2) = \tfrac{1}{2}\Gamma(l+\tfrac{1}{2}N+p+\tfrac{1}{2}+p'). \tag{43}$$

Using this result plus the identity

$$\sum_{p'=0}^{n'} \frac{\Gamma(-n'+p')\Gamma(l+\frac{1}{2}N)\Gamma(l+\frac{1}{2}N+p+p'+\frac{1}{2})}{\Gamma(-n')\Gamma(l+\frac{1}{2}N+p')p'!}$$
$$= \Gamma(l+\tfrac{1}{2}N+p+\tfrac{1}{2})\,{}_2F_1(-n';\ l+\tfrac{1}{2}N+p+\tfrac{1}{2};\ l+\tfrac{1}{2}N;\ 1), \tag{44}$$

as well as Gauss' summation theorem [5]

$$\sum_{p'=0}^{n'} \frac{\Gamma(-n'+p')\Gamma(l+\frac{1}{2}N)\Gamma(l+\frac{1}{2}N+p+\frac{1}{2}+p')}{\Gamma(-n')\Gamma(l+\frac{1}{2}N+p')p'!}$$
$$= \frac{\Gamma(l+\frac{1}{2}N+p+\frac{1}{2})\Gamma(l+\frac{1}{2}N)\Gamma(n'-p-\frac{1}{2})}{\Gamma(l+\frac{1}{2}N+n')\Gamma(-p-\frac{1}{2})}, \tag{45}$$

one finds

$$\langle nlm\,|\,r\,|\,n'lm\rangle = \frac{1}{\Gamma^2(l+\frac{1}{2}N)}\left[\frac{\Gamma(n+l+\frac{1}{2}N)\Gamma(n'+l+\frac{1}{2}N)}{n!\,n'!}\right]^{1/2}$$
$$\times \sum_{p=0}^{\infty} \frac{[\Gamma(-n+p)\Gamma(l+\frac{1}{2}N)\Gamma(l+\frac{1}{2}N+\frac{1}{2}+p)\Gamma(l+\frac{1}{2}N)\Gamma(n'-p-\frac{1}{2})}{\Gamma(-n)\Gamma(l+\frac{1}{2}N+p)p!\,\Gamma(l+\frac{1}{2}N+n')\Gamma(-p-\frac{1}{2})]}. \tag{46}$$

Then using $\Gamma(n-z)/\Gamma(-z) = (-1)^n\Gamma(z+1)/\Gamma(z+1-n)$ [3] and identifying the ${}_3F_2$ function in the resulting sum, one obtains the desired result, equation (32).

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